

# «beta»-Alanine, N-(2-furoyl)-, butyl ester

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C12H17NO4/c1-2-3-8-17-11(14)6-7-13-12(15)10-5-4-9-16-10/h4-5,9H,2-3,6-8H |
| <b>InchiKey:</b>            | ZEGDVBMUAMJTMN-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C12H17NO4   |
| <b>SMILES:</b>              | CCCCOC(=O)CCNC(=O)c1ccco1   |
| <b>Mol. weight [g/mol]:</b> | 239.27  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -6.92   |        | Crippen Method |
| logp          | 1.743   |        | Crippen Method |
| mcvol         | 185.340 | ml/mol | McGowan Method |
| rinpol        | 1902.00 |        | NIST Webbook   |
| rinpol        | 1902.00 |        | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321974&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321974&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mcvol:</b>   | McGowan's characteristic volume     |
| <b>rinpol:</b>  | Non-polar retention indices         |

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